Development & Application of Advanced Plume-in-Grid (PiG) Multi-Pollutant Models

Prakash Karamchandani, Krish Vijayaraghavan,
Shu-Yun Chen & Christian Seigneur
AER, Inc., San Ramon, CA

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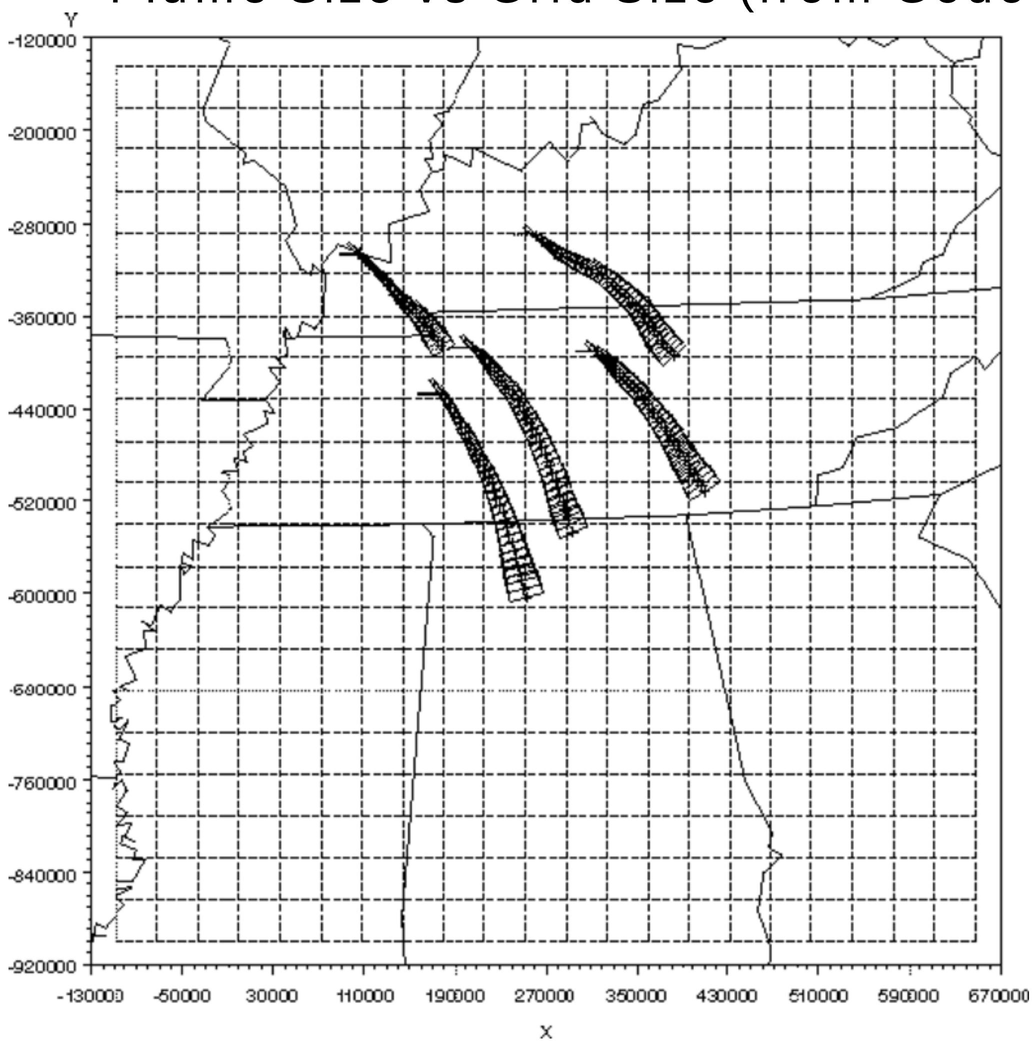
Why Use Plume-in-Grid Approach?

Plume Size vs Grid Size (from Godowitch, 2004)

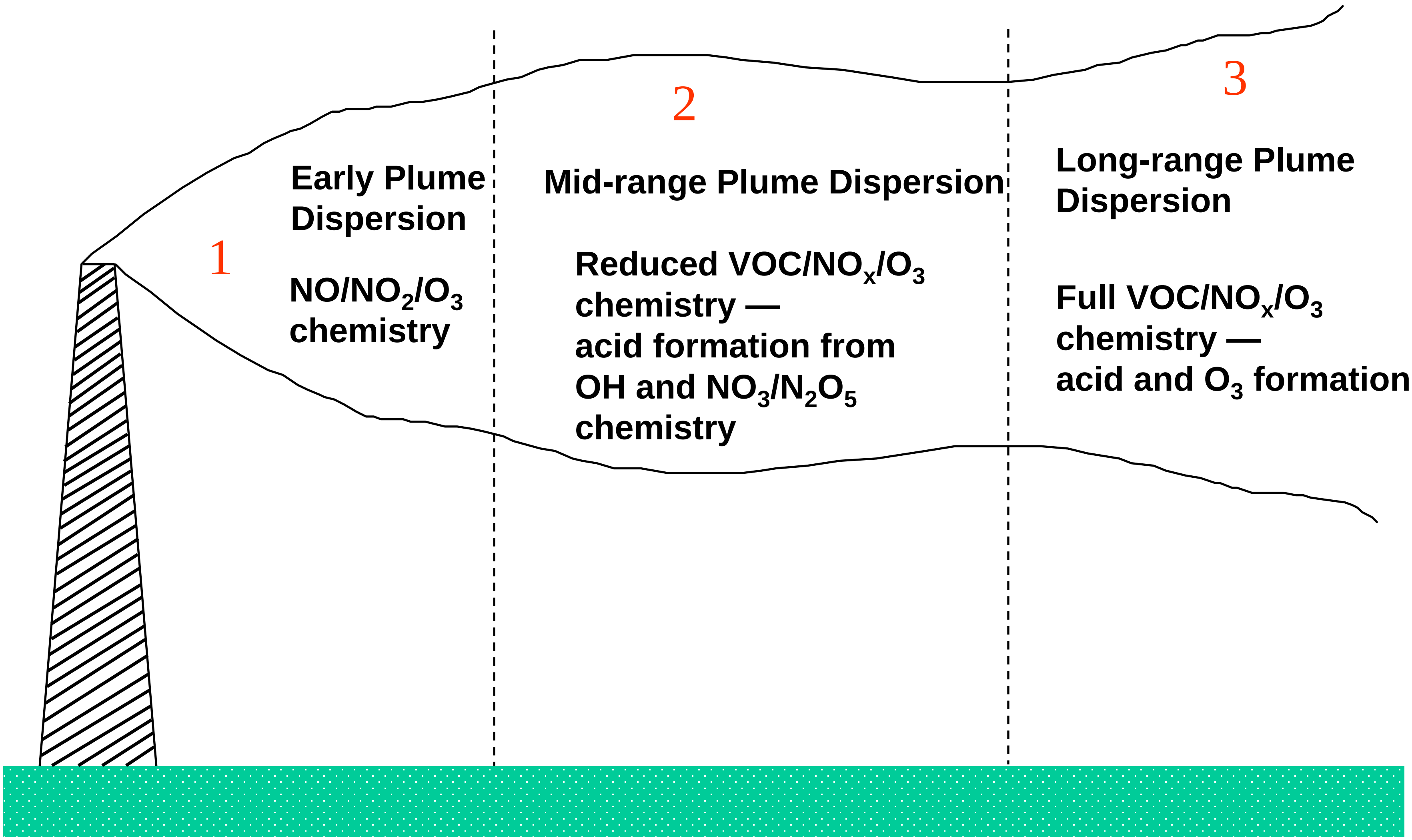


Limitations of Purely Grid-Based Approach

- **Artificial dilution of stack emissions**
- **Unrealistic near-stack plume concentrations**
- **Incorrect representation of plume chemistry**
- **Incorrect representation of plume transport**

Subgrid-scale representation of plumes addresses these limitations

Plume Chemistry & Relevance to Ozone & PM Modeling



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PiG Modeling

- PiG model consists of a reactive plume model embedded within a 3-D grid model
  - Plume model captures local variability in concentrations near sources with full treatment of chemistry
  - Grid model provides continuously evolving background concentrations
  - Grid model concentrations are adjusted at large downwind distances when the plume size is commensurate with the grid size: plume material is “handed over” to grid model

History of PiG Modeling

- Began in the 1980s, focusing on ozone (PiG version of UAM was called PARIS - Plume-Airshed Reactive-Interacting System)-Seigneur et al., 1983, Atmos. Environ.
- Early models were overly simplified
  - No treatment of wind shear or plume overlaps
  - No treatment of effect of atmospheric turbulence on chemical kinetics
  - Simplified treatment of chemistry in some models
- The development of a state-of-the-science PiG model for ozone was initiated in 1997 under EPRI sponsorship

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Advanced PiG Model

- Embedded Plume Model: SCICHEM (state-of-the science treatment of stack plumes at the sub-grid scale)-developed by L-3 Communications/Titan and AER (Karamchandani et al., 2000, ES&T).
  - SCICHEM is based on SCIPUFF, an alternative model recommended by EPA on a case-by-case basis for regulatory applications (also used by DTRA and referred to as HPAC)
  - Three-dimensional puff-based model, with second-order closure approach for plume dispersion and treatment of puff splitting and merging
  - SCICHEM adds full chemistry mechanism (e.g., CBM-IV) to SCIPUFF

Advanced PiG Model

- SCICHEM was first embedded in MAQSIP, the precursor to the U.S. EPA Model, CMAQ
- In 2000, AER incorporated SCICHEM into CMAQ (Karamchandani et al., 2002, JGR)
- The model is called CMAQ-APT (Advanced Plume Treatment)

CMAQ-APT Applications for Ozone

- Eastern United States with two nested grid domains (12 and 4 km resolution), July 1995 (Karamchandani et al., 2002, JGR)
- Central California (4 km resolution), July-August 2000 (Vijayaraghavan et al., 2006, Atmos. Environ.)
- Key conclusion from Eastern U.S. application: for isolated point sources, CMAQ-APT predicts lower O_3 and HNO_3 formation compared to the base model

Addition of PM Treatment in the PiG Model

- PM and aqueous-phase chemistry treatments were added in 2004-2005 (Karamchandani et al., 2006, Atmos. Environ.)
- Two versions:
  - EPA treatment of PM (CMAQ-AERO3-APT)
  - MADRID treatment of PM (CMAQ-MADRID-APT), developed by AER

MADRID: Model of Aerosol Dynamics, Reaction, Ionization and Dissolution (Zhang et al., 2004, JGR)

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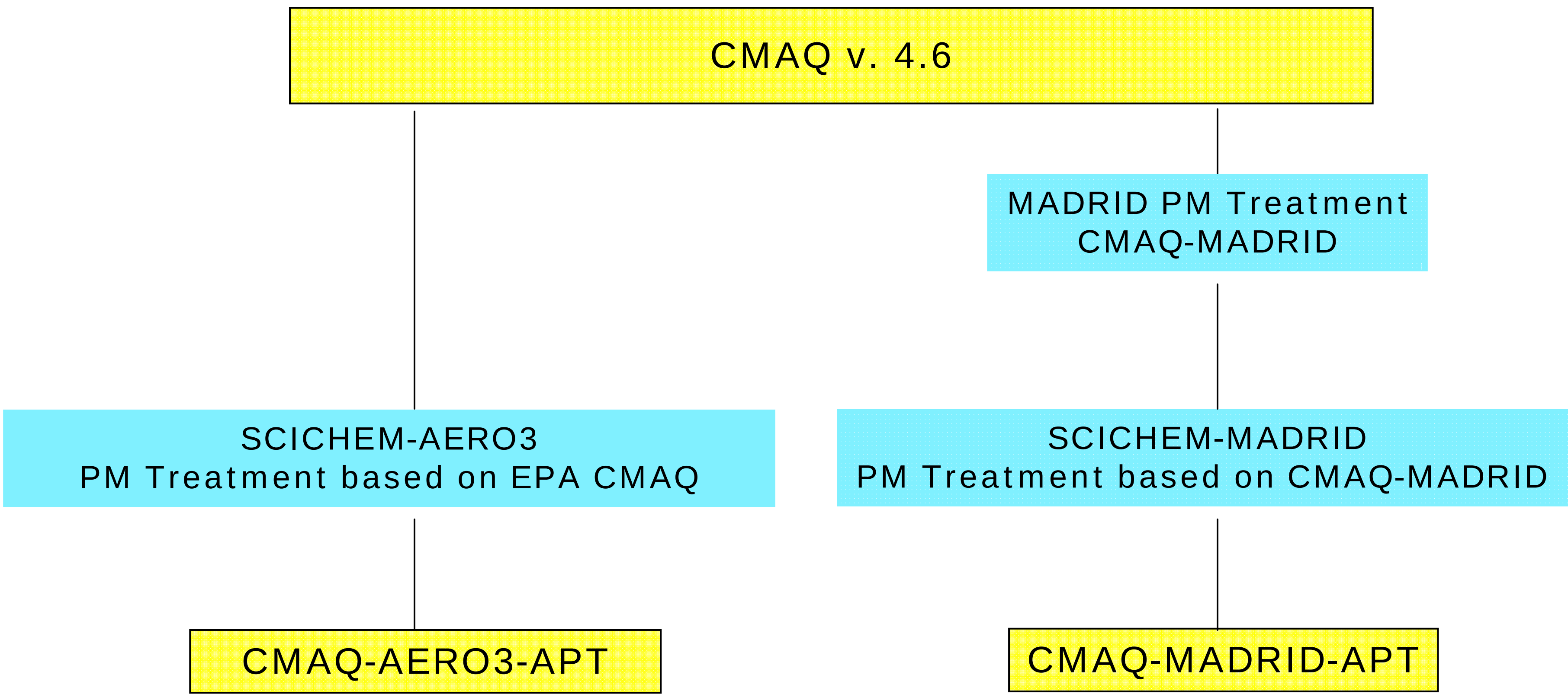
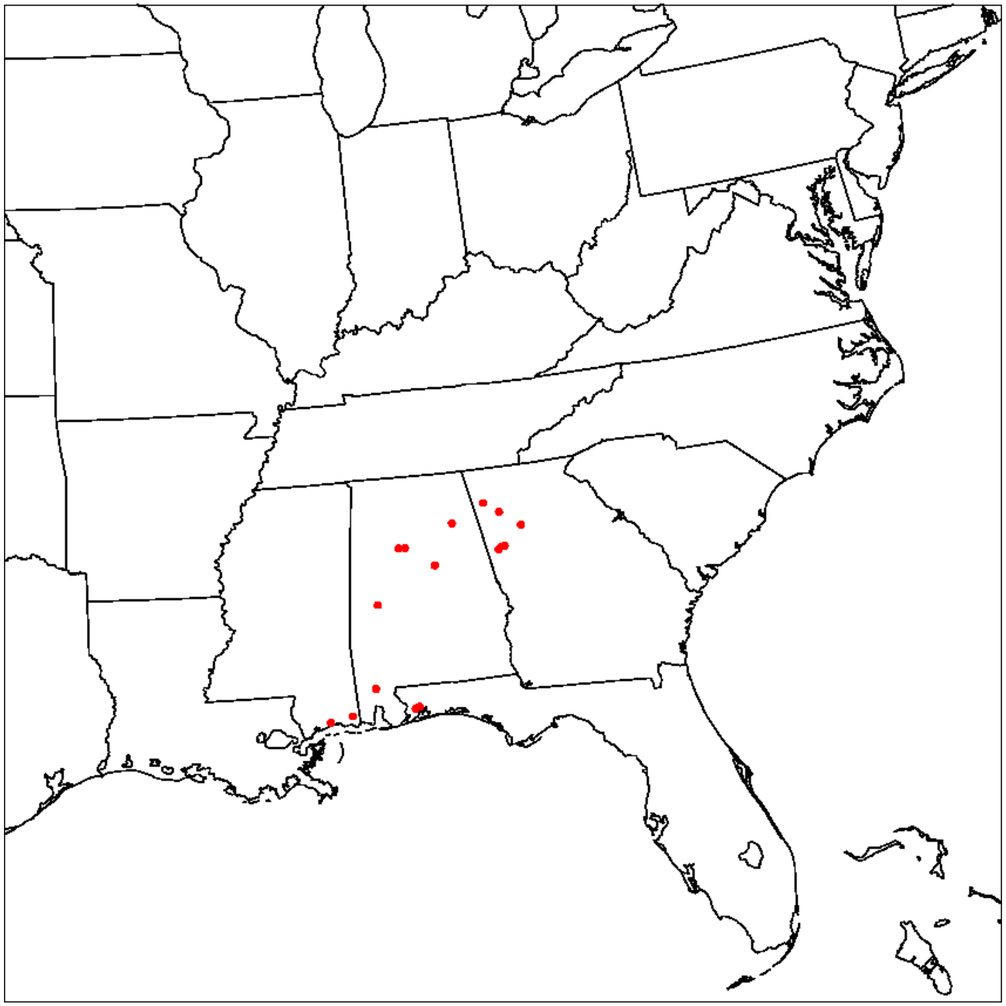
Model Components



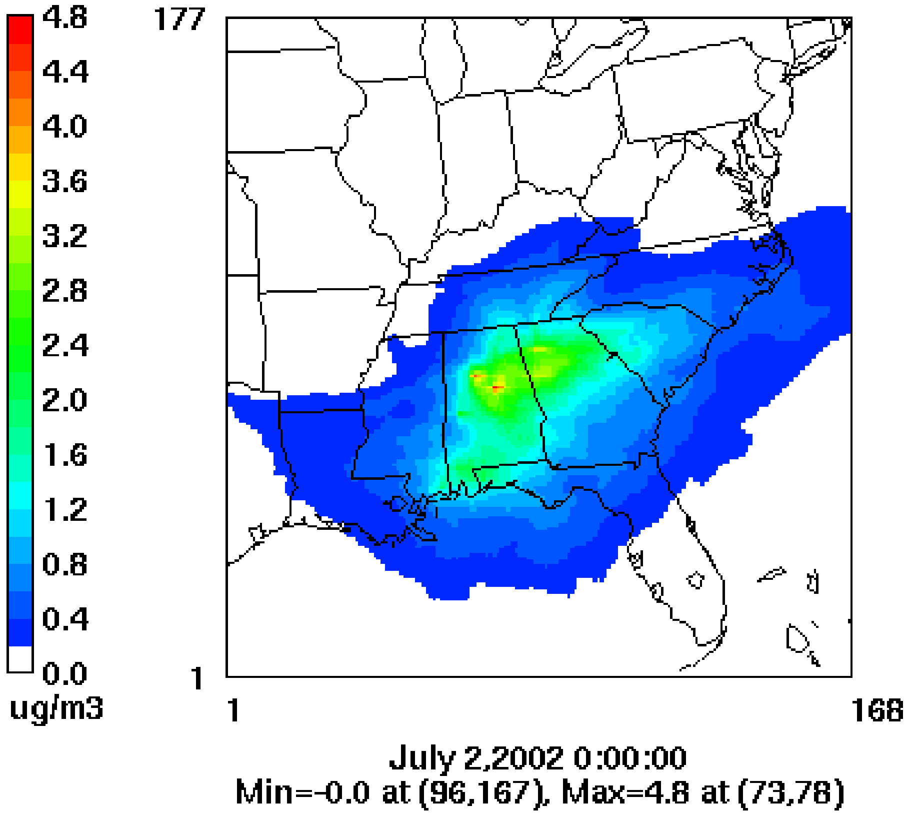
Application to Southeastern U.S.

- Study designed to supplement RPO modeling being conducted by the Visibility Improvement State and Tribal Association of the Southeast (VISTAS)
- 2 months simulated (January and July 2002) with Base CMAQ v 4.4 and CMAQ-APT-PM
- 14 power plant plumes explicitly simulated with plume-in-grid approach
- Model performance: Base CMAQ vs. CMAQ-APT-PM
- Power plant contributions to $PM_{2.5}$ components calculated and compared for Base CMAQ and CMAQ-APT-PM

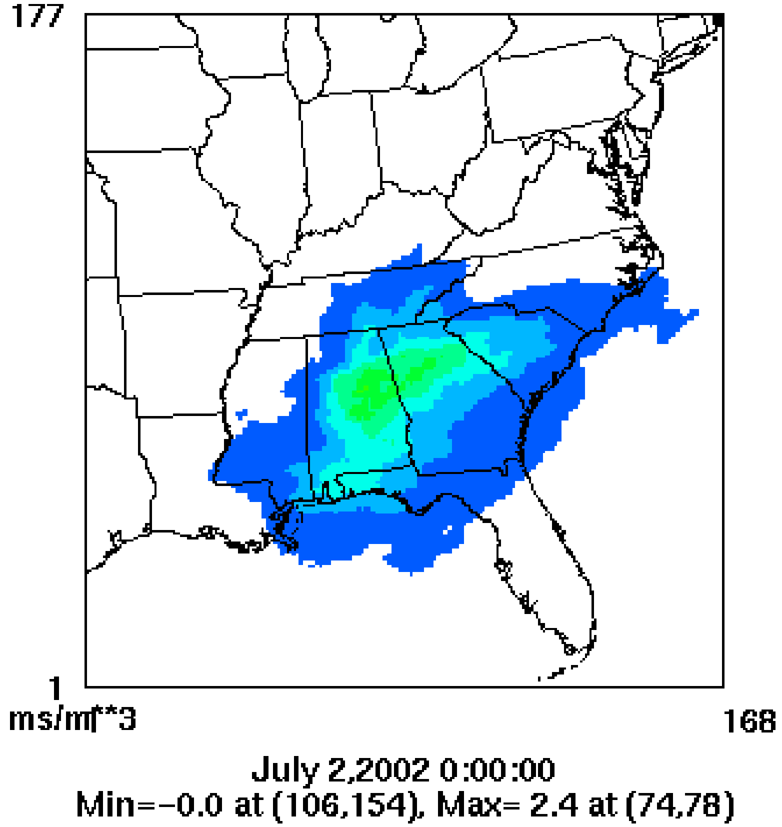
Modeling Domain and Locations of PiG sources



Power-Plant Contributions to Average July $PM_{2.5}$ Sulfate Concentrations

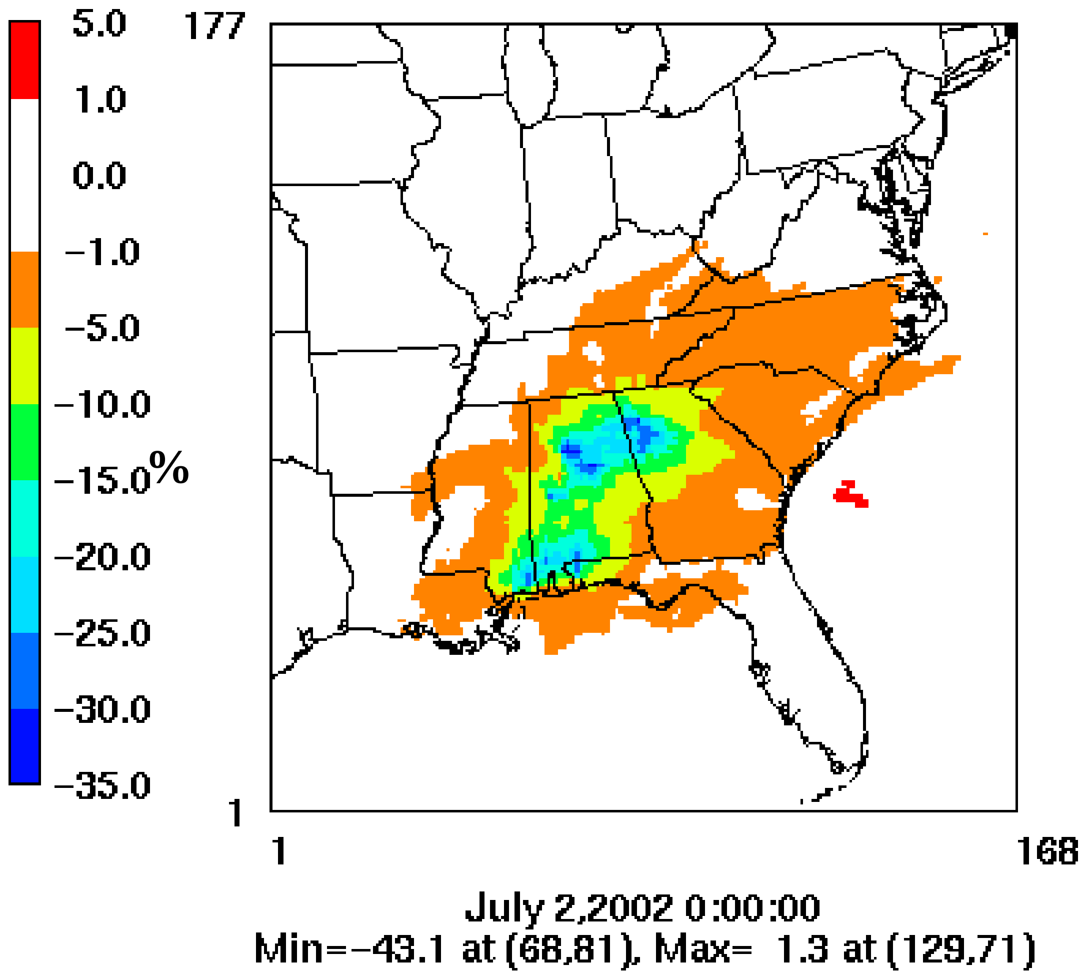


Base CMAQ



CMAQ-AERO3-APT

Change in Power-Plant Contributions to $PM_{2.5}$ Sulfate Concentrations When a Plume-in-Grid Approach is Used



Predicted power plant contributions to sulfate are lower when a PiG treatment is used

Conclusions from CMAQ-AERO3-APT Application

- Using a purely gridded approach will typically overestimate power plant contributions to PM because SO_2 to sulfate and NO_x to nitrate conversion rates are overestimated
- Plume-in-grid PM modeling provides a better representation of the near-source transport and chemistry of point source emissions and their contributions to $PM_{2.5}$ concentrations
- CMAQ-AERO3-APT predicts lower power plant contributions than base CMAQ to local and regional sulfate and total nitrate, particularly in summer

Addition of Mercury Treatment in the PiG Model

- Implementation of mercury modules in CMAQ-MADRID-APT was completed in 2006 (Karamchandani et al., 2006, 5th Annual CMAS Conference)
- Application of CMAQ-MADRID-APT (with Hg) to the southeastern U.S. (12 km grid resolution) for 2002
- Application of CMAQ-MADRID-APT (with Hg) to continental U.S. (36 km grid resolution) for 2001 (Vijayaraghavan et al., 2008, JGR)

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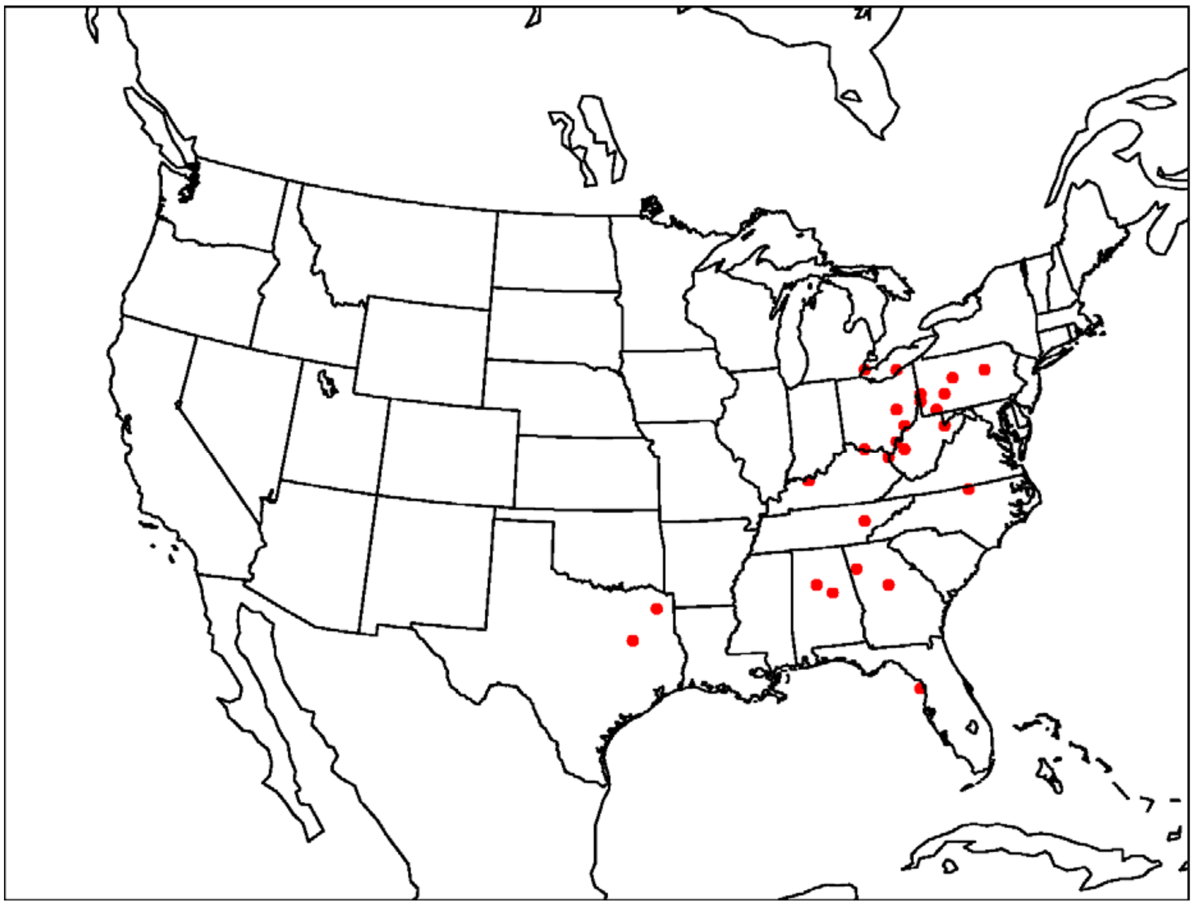
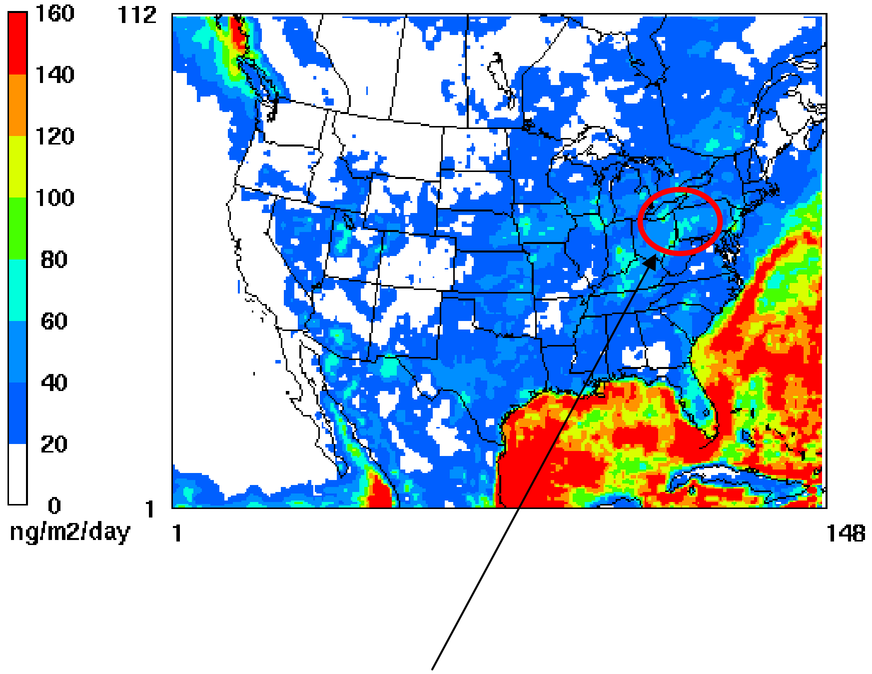
Continental U.S. Application for 2001



- 30 power plants with highest Hg^{II} emissions
- 36 km grid

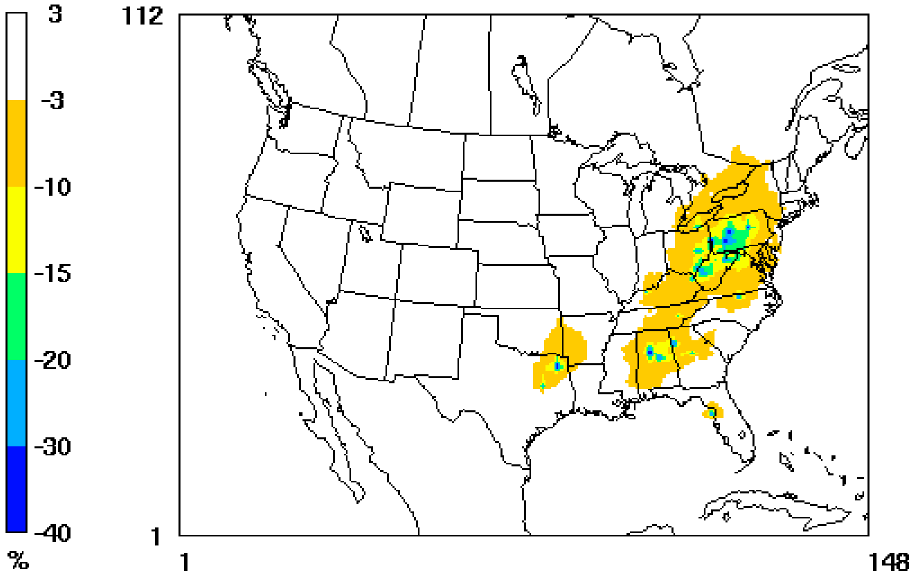
Mercury Wet Deposition Flux in Aug-Sep. 2001

Grid Model



The model over-predicts wet deposition in Pennsylvania

% Change due to APT



The advanced plume treatment corrects some of the overprediction

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Sub-Grid Scale Modeling of Air Toxics Concentrations Near Roadways

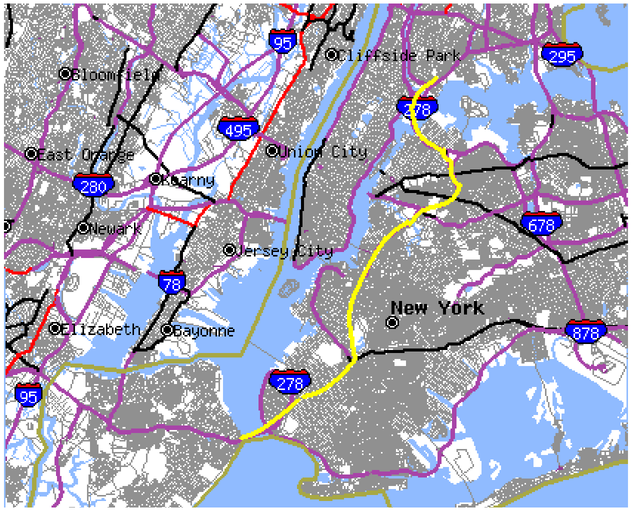
- Population exposure to hazardous air pollutants (HAPs) is an important health concern
- Exposure levels near roadways are factors of 10 larger than in the background–models need to capture spatial variability in exposure levels
- Many of the species of interest are chemically reactive–e.g., formaldehyde, 1,3-butadiene, acetaldehyde–models need to treat the chemistry of these species
- Traditional modeling approaches are inadequate to provide both chemistry treatment and fine spatial resolution

PiG Modeling for Roadway Emissions

- Based on CMAQ-APT
- Prototype version developed in 2007 (Karamchandani et al., 2008, Env. Fluid Mech.):
  - simulates near-source CO and benzene concentrations from roadway emissions
  - chemistry is switched off
  - roadway emissions treated as series of area sources along the roadway with initial size equal to the roadway width
- Concentrations calculated at discrete receptor locations by combining incremental puff concentrations with the grid-cell average background concentration

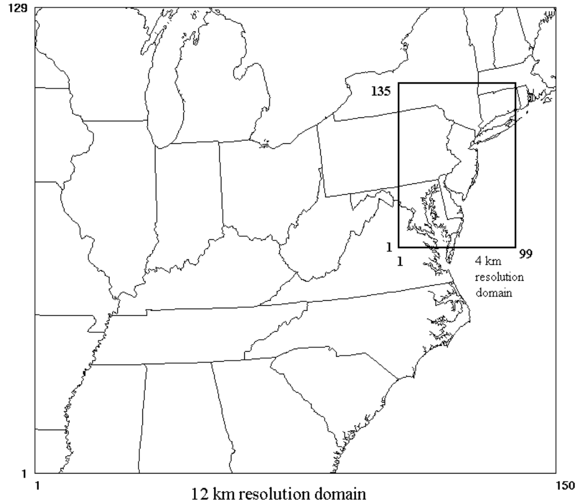
Model Application

- Busy interstate highway in New York City (I278)

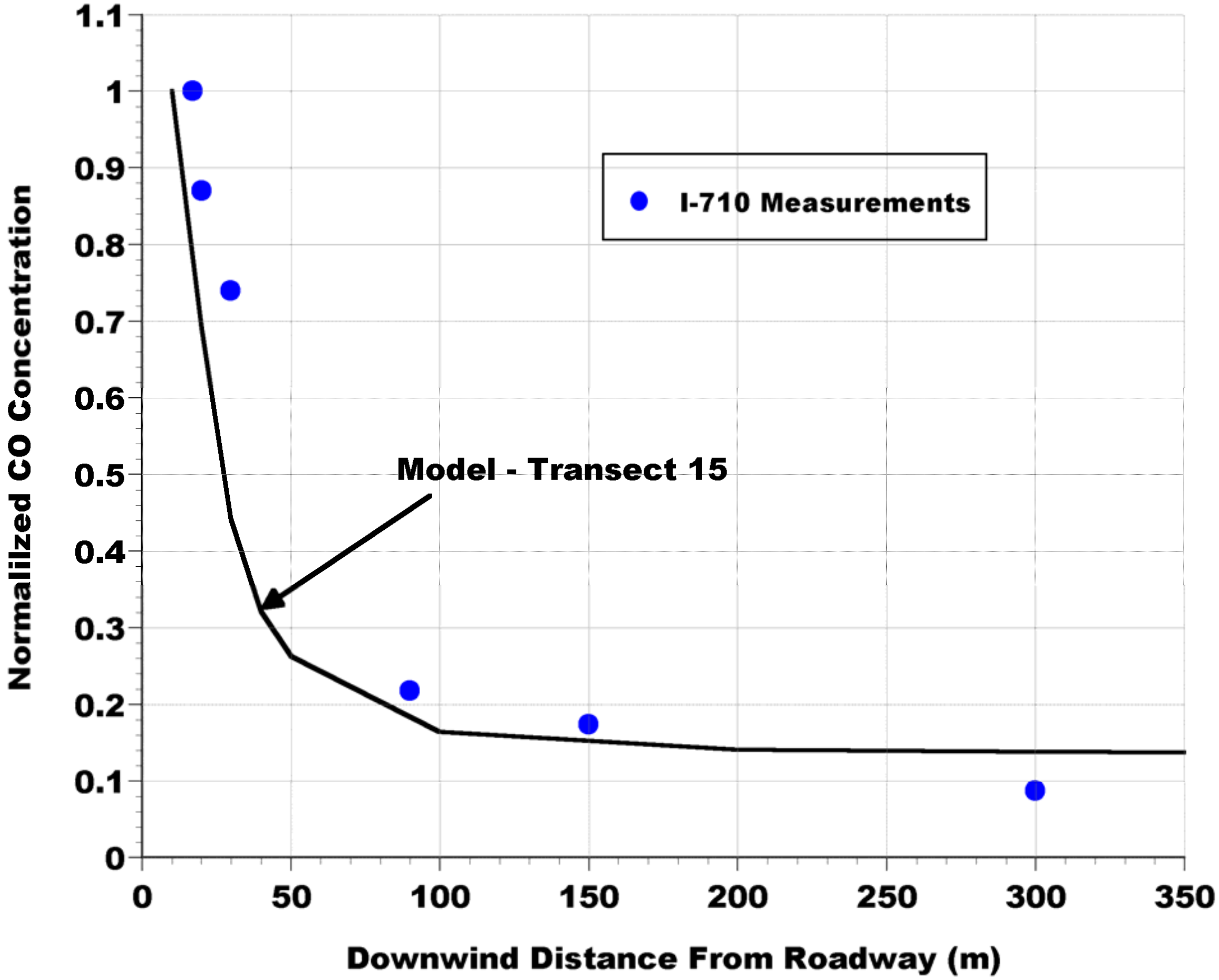


- July 11-15, 1999 period of NARSTO/Northeast Program

- Grid model domain



Qualitative Evaluation of CO Concentrations



- Results compared with CO concentration profiles measured in Los Angeles by Zhu et al. (2002), Atmos. Environ.

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PiG Modeling Constraints

- Can be computationally expensive if a large number of point sources are treated with the puff model – computational requirements increase by a factor of two to three for 50 to 100 sources
- Point sources have to be selected carefully to limit the number of sources treated
- To obtain results in a reasonable amount of time, annual simulations are usually conducted by dividing the calendar year into quarters and simulating each quarter on different processors or machines
- Parallel version of code can address these constraints

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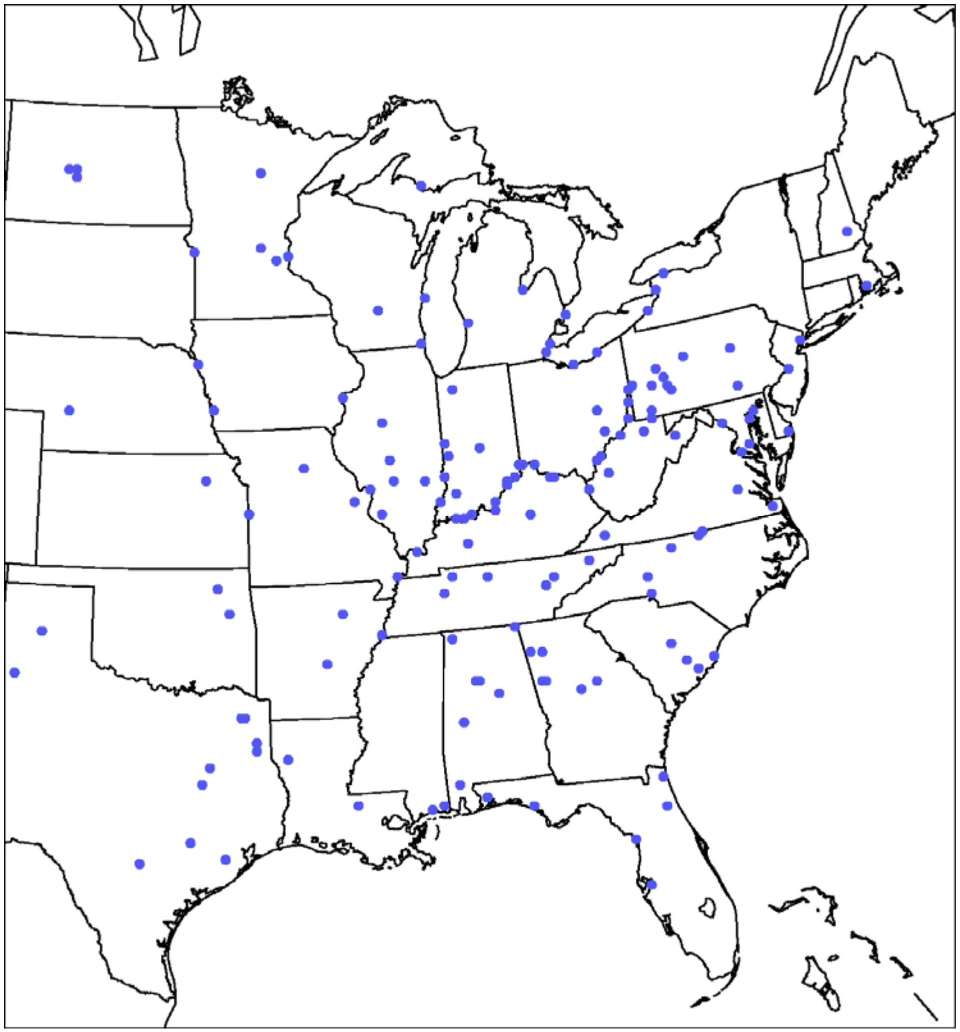
Parallelization of PiG Model

- Development of parallel version of CMAQ-MADRID-APT completed in late 2007
- On a 4-processor machine, the parallel version is about 2.5 times faster than the single-processor version
- On-going project to apply the model to the central and eastern United States at 12 km resolution and to evaluate it with available data
  - Over 150 point sources explicitly treated with APT
  - Annual actual and typical simulations for 2002
  - Future year emission scenarios
  - Other emission sensitivity scenarios

Ongoing Application of Parallel PiG Model



- 12 km grid resolution
- 243 x 246 x 19 grid cells
- Over 150 PiG sources

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Acknowledgments

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- Data Sources:
  - VISTAS
  - Atmospheric Research & Analysis, Inc. (ARA)
  - Georgia Environmental Protection Division (GEPD)